

Perfluorovaleric acid

2706-90-3 | DTXSID6062599

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.35e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 3.00e-01

Confidence level: 4.98e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Fluopropanate-sodium

Measured: 1.31e-01

Predicted: 4.65e-01

[Image not found](#)

Acetic acid, trifluoro-

Measured: 8.77

Predicted: 4.36

[Image not found](#)

2,2,2-Trifluoroethanol

Measured: 10.0

Predicted: 6.34